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**Approximating Multivariate Normal
Orthant Probabilities
ONR Technical Report**

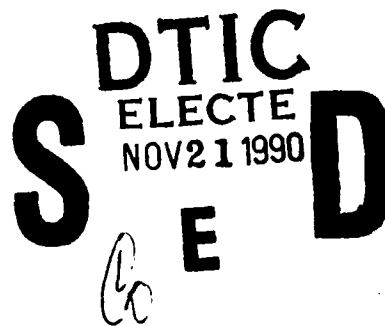
Robert D. Gibbons
University of Illinois at Chicago

R. Darrell Bock
University of Chicago

Donald R. Hedeker
University of Illinois at Chicago

May 1990

Dr. R.D. Gibbons
Biometric Laboratory
Illinois State Psychiatric Institute,
1601 W. Taylor St., Chicago, IL 60612, USA.



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REPORT DOCUMENTATION PAGE

Form Approved
OMB No 0704-0188

REPORT SECURITY CLASSIFICATION Unclassified		1b RESTRICTIVE MARKINGS	
SECURITY CLASSIFICATION AUTHORITY		3 DISTRIBUTION AVAILABILITY OF REPORT Approved for public release; distribution unlimited	
DECLASSIFICATION/DOWNGRADING SCHEDULE			
PERFORMING ORGANIZATION REPORT NUMBER(S) Biometric Lab Report #90-1		5 MONITORING ORGANIZATION REPORT NUMBER(S)	
NAME OF PERFORMING ORGANIZATION University of Illinois	6b OFFICE SYMBOL (if applicable)	7a NAME OF MONITORING ORGANIZATION Cognitive Science Research Program Office of Naval Research (Code 1142CS)	
ADDRESS (City, State, and ZIP Code) Illinois State Psychiatric Institute 529W 601 West Taylor Street Chicago, Illinois 60612		7b ADDRESS (City, State, and ZIP Code) 800 N. Quincy Street Arlington, Virginia 22217-5000	
NAME OF FUNDING/SPONSORING ORGANIZATION	8b OFFICE SYMBOL (if applicable)	9 PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER N 00014-89-J-1104	
ADDRESS (City, State, and ZIP Code)		10 SOURCE OF FUNDING NUMBERS	
		PROGRAM ELEMENT NO 61153N	PROJECT NO RR042046
		TASK NO RR04204-01	WORK UNIT ACCESSION NO 4421553

TITLE (Include Security Classification)

Approximating Multivariate Normal Orthant Probabilities

PERSONAL AUTHOR(S)

Robert D. Gibbons, R. Darrell Bock and Donald Hedeker

TYPE OF REPORT Interim	13b TIME COVERED FROM 6/01/89 TO 6/01/90	14 DATE OF REPORT (Year, Month, Day) June 1, 1990	15 PAGE COUNT
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SUPPLEMENTARY NOTATION

To be submitted for publication in Technometrics

16a SUBJECT TERMS (Continue on reverse if necessary and identify by block number)		
FIELD	GROUP	SUB GROUP
25	09	

ABSTRACT (Continue on reverse if necessary and identify by block number)

The probability integral of the multivariate normal distribution has received considerable attention since Sheppard (1900) and Pearson (1901) published their seminal work on the bivariate normal distribution. In the general case, we are concerned with evaluating

$$F_n(h_1, h_2, \dots, h_n; \{\rho_{ij}\}) = \int_{-\infty}^{h_1} \int_{-\infty}^{h_2} \dots \int_{-\infty}^{h_n} f(x_1, x_2, \dots, x_n; \{\rho_{ij}\}) dx_1 \dots dx_n$$

where $\{\rho_{ij}\}$ represents the $n \times n$ symmetric correlation matrix of the x_i 's, and $f(x_1, x_2, \dots, x_n; \{\rho_{ij}\})$ is the standardized multivariate normal density function. Direct evaluation of F_n is only possible for special cases of $\{\rho_{ij}\}$. For example, Dunnett and Sobel (1955) have shown that when $\rho_{ij} = \alpha_i \alpha_j (i \neq j)$, where $|\alpha_i| \leq 1$, then

DISTRIBUTION AVAILABILITY OF ABSTRACT <input checked="" type="checkbox"/> UNCLASSIFIED/UNLIMITED <input type="checkbox"/> SAME AS RPT <input type="checkbox"/> DTIC USERS		21 ABSTRACT SECURITY CLASSIFICATION Unclassified	
NAME OF RESPONSIBLE INDIVIDUAL Dr. Charles Davis		22a TELEPHONE (Include Area Code) 202/696-4046	22b OFFICE SYMBOL ONR 1142PT

$$F_n(h_1, h_2, \dots, h_n; \{\rho_{ij}\}) = \int_{-\infty}^{\infty} \left[\prod_{i=1}^n \Phi \left(\frac{h_i - \alpha_i y}{\sqrt{1 - \alpha_i^2}} \right) \right] f(y) dy$$

where Φ represents the univariate normal distribution function. This special case is the basis for much of item-response theory. More recently, however, Bohrer and Schervish (1981), have developed an error bounded algorithm for evaluating F_n for general $\{\rho_{ij}\}$. Computationally, this algorithm is restricted to $n = 7$, and even at $n = 7$, it can require as much as 24 hours to compute a single probability with 10^{-3} accuracy on a computer than is capable of approximately 1-2 million scalar floating point operations per second.

The purpose of this report is to present a fast and general approximation for rectangular regions of the multivariate normal distribution function, that is based on Clark's (1961) approximation to the moments of the maximum of n jointly normal random variables. The performance of this approximation is then compared to special cases in which the exact results are known (e.g., $\rho_{ij} = \rho = .5$), cases in which the integral reduces to a unidimensional quadrature evaluation (e.g., $\rho_{ij} = \alpha_i \alpha_j$), and finally error bounded reduction formulae for $\{\rho_{ij}\}$ and $n \leq 7$.

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DTIC TAB	<input type="checkbox"/>
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Justification	
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Distribution/	
Availability Codes	
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A-1	



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The probability integral of the multivariate normal distribution has received considerable attention since Sheppard (1900) and Pearson (1901) published their seminal work on the bivariate normal distribution. In the general case, we are concerned with evaluating

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where $\{\rho_{ij}\}$ represents the $n \times n$ correlation matrix of the x_i 's, and $f(x_1, x_2, \dots, x_n; \{\rho_{ij}\})$ is the standardized multivariate normal density function. Direct evaluation of F_n is only possible for special cases of $\{\rho_{ij}\}$. For example, Dunnett and Sobel (1955) have shown that when $\rho_{ij} = \alpha_i \alpha_j (i \neq j)$, where $|\alpha_i| \leq 1$, then

$$F_n(h_1, h_2, \dots, h_n; \{\rho_{ij}\}) = \int_{-\infty}^{\infty} \left[\prod_{i=1}^n \Phi \left(\frac{h_i - \alpha_i y}{\sqrt{1 - \alpha_i^2}} \right) \right] f(y) dy$$

where Φ represents the univariate normal distribution function. This special case is the basis for much of modern psychometric theory. More recently, however, Bohrer and Schervish (1981), have developed an error-bounded algorithm for evaluating F_n for general $\{\rho_{ij}\}$. Computationally, this algorithm is restricted to $n = 7$, and even at $n = 7$, it can require as much as 24 hours to compute a single probability with 10^{-3} accuracy on a computer than is capable of approximately 1-2 million scalar floating point operations per second.

The purpose of this report is to present a fast and general approximation for rectangular regions of the multivariate normal distribution function based on Clark's (1961) approximation to the moments of the maximum of n jointly normal random variables. The performance of this approximation compared to special cases in which the exact results are known and error-bounded reduction formulae show the accuracy of the approximation to be adequate for many practical applications where multivariate normal probabilities are required. (kP)

1 Introduction

The probability integral of the multivariate normal distribution has received considerable attention since Sheppard (1900) and Pearson (1901) published their seminal work on the bivariate normal distribution. In the general case, we are concerned with evaluating

$$F_n(h_1, h_2, \dots, h_n; \{\rho_{ij}\}) = \int_{-\infty}^{h_1} \int_{-\infty}^{h_2} \dots \int_{-\infty}^{h_n} f(x_1, x_2, \dots, x_n; \{\rho_{ij}\}) dx_1 \dots dx_n \quad (1)$$

where $\{\rho_{ij}\}$ represents the $n \times n$ symmetric correlation matrix of the x_i 's, and $f(x_1, x_2, \dots, x_n; \{\rho_{ij}\})$ is the standardized multivariate normal density function. Direct evaluation of F_n is only possible for special cases of $\{\rho_{ij}\}$. For example, Dunnett and Sobel (1955) have shown that when $\rho_{ij} = \alpha_i \alpha_j (i \neq j)$, where $|\alpha_i| \leq 1$, then

$$F_n(h_1, h_2, \dots, h_n; \{\rho_{ij}\}) = \int_{-\infty}^{\infty} \left[\prod_{i=1}^n \Phi \left(\frac{h_i - \alpha_i y}{\sqrt{1 - \alpha_i^2}} \right) \right] f(y) d(y) \quad (2)$$

where Φ represents the univariate normal distribution function. The probability in equation (2) can be approximated to any practical degree of accuracy using Gauss-Hermite quadrature (Stroud and Secrest, 1966). It should be noted that when $\rho_{ij} = \rho$ for all i, j , then

$$F_n(h, h, \dots, h; \{\rho\}) = \int_{-\infty}^{\infty} \left[\Phi^n \left(\frac{h + \rho^{1/2} y}{\sqrt{1 - \rho}} \right) \right] f(y) d(y) \quad (3)$$

and if $\rho = .5$ and $h = 0$,

$$F_n(0, 0, \dots, 0; \{.5\}) = \frac{1}{n+1} \quad (4)$$

More recently, however, Bohrer and Schervish (1981), have developed an error-bounded algorithm for evaluating F_n for general $\{\rho_{ij}\}$. Computationally, this algorithm is restricted to $n = 7$, and even at $n = 7$, it can require as much as 24 hours to compute a single probability with 10^{-3} accuracy on a computer that is capable of approximately 1-2 million scalar floating point operations per second. It is unclear whether vectorization of this algorithm is possible, so that the greatly increased speeds of parallel computing environments could be exploited (e.g., 20-80 million floating point instructions per second). Even still, it is unlikely that this algorithm would be computationally tractable for $n > 10$.

An alternate approach to approximating F_n , can be obtained by noting that,

$$F_n = Pr(x_1 \leq h_1, x_2 \leq h_2, \dots, x_n \leq h_n) \quad (5)$$

If $h_1 \dots h_n = h = 0$, and the x_i follow a standardized multivariate normal distribution, F_n^0 is a so-called "orthant" probability. Note, however, that this orthant probability is equivalent to

$$F_n^0 = Pr\{max(x_1, \dots, x_n) \leq 0\} \quad (6)$$

If $max(x_1, \dots, x_n)$ were normally distributed, which it clearly is not, with mean $E[max(x_1, \dots, x_n)]$ and variance $V[max(x_1, \dots, x_n)]$, then,

$$F_n^0 = \Phi \left[\frac{h - E[max(x_1, \dots, x_n)]}{\sqrt{V[max(x_1, \dots, x_n)]}} \right] \quad (7)$$

where in this case $h = 0$. For the more general rectangular region case of h_i , we could set $h = 0$ and subtract h_i from the mean values of each of the x_i , which to this point have been expressed in standardized form.

To use this algorithm, we must first have an accurate method of computing the first two moments of $max(x_1, \dots, x_n)$ where the x_i have a joint multivariate normal distribution with general correlation $\{\rho_{ij}\}$, and some bound on the error introduced by assuming that $max(x_1, \dots, x_n)$ has a normal distribution. Such an approximation has been described by Clark (1961), and in the following, we describe its use in connection with evaluating $F_n(x_1, x_2, \dots, x_n; \{\rho_{ij}\})$. We begin by reviewing Clark's original formulae.

2 The Clark Algorithm

Let any three successive components from an n -variate vector, y_i , be distributed:

$$\begin{bmatrix} y_i \\ y_{i+1} \\ y_{i+2} \end{bmatrix} \sim N \left(\begin{bmatrix} \mu_i \\ \mu_{i+1} \\ \mu_{i+2} \end{bmatrix}, \begin{bmatrix} \sigma_i^2 & & \\ \sigma_i \sigma_{i+1} \rho_{i,i+1} & \sigma_{i+1}^2 & \\ \sigma_i \sigma_{i+2} \rho_{i,i+2} & \sigma_{i+1} \sigma_{i+2} \rho_{i+1,i+2} & \sigma_{i+2}^2 \end{bmatrix} \right)$$

Let $\tilde{y}_i = \max(y_i) = y_i$, and compute the probability that $y_{i+1} > \tilde{y}_i$ as follows:

$$\text{set} \quad z_{i+1} = (\mu_i - \mu_{i+1})/\zeta_{i+1},$$

$$\text{where} \quad \zeta_{i+1}^2 = \sigma_i^2 + \sigma_{i+1}^2 - 2\sigma_i \sigma_{i+1} \rho_{i,i+1}.$$

$$\begin{aligned} \text{Then } P(y_{i+1} > \tilde{y}_i) &= P(y_{i+1} - \tilde{y}_i > 0) \\ &= \Phi(-z_{i+1}) \end{aligned}$$

the value of the univariate normal distribution function at the standard deviate $-z_{i+1}$.

Now let $\tilde{y}_{i+1} = \max(y_i, y_{i+1})$ and assume (as an approximation) that $(y_{i+2}, \tilde{y}_{i+1})$ is bivariate normal with means,

$$\begin{aligned}\mu(y_{i+2}) &= \mathcal{E}(y_{i+2}) = \mu_{i+2} \\ \mu(\tilde{y}_{i+1}) &= \mathcal{E}(\tilde{y}_{i+1}) = \mu_i \Phi(z_{i+1}) + \mu_{i+1} \Phi(-z_{i+1}) + \zeta_{i+1} \phi(z_{i+1}),\end{aligned}\quad (8)$$

variances

$$\begin{aligned}\sigma^2(y_{i+2}) &= \mathcal{E}(y_{i+2}^2) - \mathcal{E}^2(y_{i+2}) = \sigma_{i+2}^2 \\ \sigma^2(\tilde{y}_{i+1}) &= \mathcal{E}(\tilde{y}_{i+1}^2) - \mathcal{E}^2(\tilde{y}_{i+1}) = \sigma_{i+2}^2.\end{aligned}\quad (9)$$

where

$$\mathcal{E}(\tilde{y}_{i+1}^2) = (\mu_i^2 + \sigma_i^2) \Phi(z_{i+1}) + (\mu_{i+1}^2 + \sigma_{i+1}^2) \Phi(-z_{i+1}) + (\mu_i + \mu_{i+1}) \zeta_{i+1} \phi(z_{i+1}). \quad (10)$$

and correlation

$$\rho(\tilde{y}_{i+1}, y_{i+2}) = \frac{\sigma_i \rho_{i,i+2} \Phi(z_{i+1}) + \sigma_{i+1} \rho_{i+1,i+2} \Phi(-z_{i+1})}{\sigma(\tilde{y}_{i+1})}. \quad (11)$$

Then,

$$P(y_{i+2} = \max(y_i, y_{i+1}, y_{i+2})) = P((y_{i+2} - y_{i+1} > 0) \cap (y_{i+2} - y_i > 0)) \quad (12)$$

is approximated by

$$\begin{aligned}P(y_{i+2} > \tilde{y}_{i+1}) &= P(y_{i+2} - \tilde{y}_{i+1} > 0) \\ &= \Phi\left(\frac{\mu_{i+2} - \mu(\tilde{y}_{i+1})}{\sqrt{\sigma_{i+2}^2 + \sigma^2(\tilde{y}_{i+1}) - 2\sigma_{i+2}\sigma(\tilde{y}_{i+1})\rho(\tilde{y}_{i+1}, y_{i+2})}}\right)\end{aligned}\quad (13)$$

Assuming as a working approximation that \tilde{y}_{i+1} is normally distributed with the above mean and variance, we may therefore proceed, recursively from $i = 1$ to $i = n - 1$, where y_{n+1} is an independent dummy variate with mean zero and variance zero (i.e. $y_{n+1} = 0$). Then, for example,

$$\begin{aligned}
P[y_{n+1} = \max(y_1, y_2, \dots, y_{n+1})] \\
&= P[(y_{n+1} - y_1 > 0) \cap (y_{n+1} - y_2 > 0) \cap \dots \cap (y_{n+1} - y_n > 0)] \\
&= P[(-y_1 > 0) \cap (-y_2 > 0) \cap \dots \cap (-y_n > 0)] \quad (14)
\end{aligned}$$

approximates the probability of the negative orthant of the specified multivariate normal distribution. In the case of n correlated standard normals, the negative and positive orthant probabilities are identical. The probability of any other orthant can be obtained by reversing the signs of the variates corresponding to 1's in the orthant pattern. Of course, \tilde{y}_{i+1} is not normally distributed. Errors produced by substituting normal approximations for the moments of \tilde{y}_{i+1} are discussed in the following section.

More generally, to compute a multivariate normal probability over an n dimensional rectangular region, for example,

$$\int_{-\infty}^h \int_{-\infty}^h \dots \int_{-\infty}^h f(x_1, x_2, \dots, x_n; \{\rho_{ij}\}) dx_1 \dots dx_n \quad (15)$$

we compute the negative orthant setting $\mu_{n+1} = h$. Finally, to approximate the integral for general h_i , we compute the negative orthant by setting $\mu_{n+1} = 0$ and $\mu_i = \mu_i - h_i$.

3 Accuracy of the Clark Approximation

The errors of the Clark approximation result from the replacement of non-normal distributions by normal approximations. For example, suppose that we are interested in the maximum of four standard normal variables, i.e., $\max(y_1, y_2, y_3, y_4)$. By assuming that \tilde{y}_2 is normally distributed with expected value $E[\max(y_1, y_2)]$ and variance $V[\max(y_1, y_2)]$, we can then use the moments of $\max(\tilde{y}_1, y_3)$ as an approximation for those of $\max(y_1, y_2, y_3)$. Next, we assume that \tilde{y}_3 is normally distributed with expectation and variance equal to the corresponding moments of $\max(\tilde{y}_2, y_3)$, and can therefore use the moments of $\max(\tilde{y}_3, y_4)$ as an approximation for those of $\max(y_1, \dots, y_4)$. In this example, of course, \tilde{y}_2 and \tilde{y}_3 are not normally distributed. Furthermore, this is a rare case in which the distribution of a statistical variate diverges from normality as sample size increases. Tippet (1925) first showed that skewness and kurtosis of the maximum of n standard normals goes from .019 and .62 respectively for $n = 2$ to .429 and .765 for $n = 100$ to .618 and 1.088 for $n = 1000$. In terms of expected values of n standard normal variables, the effect of this non-normality is quite small. For example, for $n = 10$, the true value is

1.5388 and the approximation yields 1.5367. Even for $n = 1000$ the expected value is 3.2414 and the approximated value is 3.2457.

The effect of non-normality on the accuracy of the approximation is also dependent on the difference between $E(\tilde{y}_{i-1}, y_i)$. For example, suppose we wish to approximate the moments of $\max(y_1, y_2)$ where y_1 and y_2 are not normally distributed. Clark (1961) points out that if the difference $E(y_1) - E(y_2)$ is large relative to the greater of $V^{1/2}(y_1)$ and $V^{1/2}(y_2)$ the random variable $\max(y_1, y_2)$ is almost identical to y_1 . Certainly the first two moments of $\max(y_1, y_2)$ would be minimally affected by replacing y_1 and y_2 by normal approximations. However if $E(y_1) - E(y_2)$ is small relative to the respective standard deviations, then the use of normal approximations could conceivably result in significant errors in the approximation of the mean and variance of their maximum.

In light of this, the following illustrations of the accuracy of the Clark approximation are, in fact, the worst case results, since they represent the case in which the expected values of the y_i are equal. These results indicate that the error bound for the Clark approximation is approximately 10^{-3} , as illustrated in the following section.

4 Illustration

To evaluate the performance of this algorithm, we have examined a series of equa-correlated multivariate normal distributions for which exact results are known (see Gupta, 1963) and those considered by Schervish (1984). Table 1A displays results for 3 to 7 equa-correlated standard normal random variables with selected values of $\rho = .2, .3, .5$ and $.9$, and upper integration bounds of 0, 1, and 2. Inspection of the tabled probabilities reveals that the Clark algorithm is generally accurate to at least 10^{-3} and that computational times are a linear function of dimensionality. The speed of the Clark algorithm does not depend on ρ . In contrast, the speed of MULNOR (Schervish, 1984) is exponentially increasing with both dimensionality and ρ . In the 7-variate normal case with $\rho_{ij} = .9$, MULNOR required almost a day to compute a probability which was accurate to 2×10^{-5} , whereas the Clark algorithm computed the same probability with 4×10^{-4} accuracy in less than three thousandths of a second. Inspection of these results and others not reported here, suggest that the accuracy of the Clark approximation increases with increasing ρ .

Table 1B displays results for orthant probabilities of higher dimensional integrals ($n = 10, 20$, and 40), for the special case of $\rho = .5$, where $F_n^0 = 1/(n+1)$. Again, results are accurate to at least 10^{-3} , and computational times are linear in n . MULNOR could not be used to evaluate integrals of this dimensionality.

Finally, Table 1C displays results for some tail probabilities of the multivariate normal distribution. In this case, the upper bound of the integration was -2.5, $n = (3, 5, 10)$, and $\rho = (.5, .9)$. These probabilities ranged from 10^{-3} to 10^{-5} and accuracy of the Clark approximation was 10^{-5} in all cases.

5 Discussion

Clark's (1961) formulae for the moments of the maximum of n correlated random normal variates can clearly be used to obtain a fast and accurate approximation to multivariate normal probabilities. Examination of a series of examples involving special cases in which the true results are known, reveals that the error bound for the approximation is approximately 10^{-3} regardless of dimensionality, and that accuracy increases with increases in $|\rho|$. These results are conservative in that we would expect the ill effect of using normal approximations to be greatest when $\mu_i = \mu, (i = 1, n)$ which is the case used in the illustrations.

In terms of computational speed, the Clark approximation is clearly unparalleled. A reasonable estimate of the speed of the Clark algorithm is given by,

$$\text{speed} = \left(\frac{.0004(n)}{\text{megaflop}} \right) \text{seconds}$$

where megaflop is the number of scalar floating point instructions per second that the computer is capable of performing.

Numerous applications of the Clark algorithm suggest themselves. Some preliminary work in this area has already been conducted by Daganzo (1984), in the context of discrete choice models of consumer behavior, and by Gibbons, Bock and Hedeker (1987) in item-response theory. Other potential applications include multivariate generalizations of probit analysis (see Ashford and Sowden, 1970 for the bivariate case), and random-effect probit models (Gibbons and Bock, 1987), where the Clark approximation was used to estimate first-order autocorrelation among the residual errors.

Another area of potential interest is in the approximation of multivariate t probabilities, which can be considered as the joint distribution of n variates $t_i = z_i/s, (i = 1, 2, \dots, n)$ where the z_i have a multivariate normal distribution with zero means and unknown variance σ^2 , and known correlation matrix $\{\rho_{ij}\}$, while $\nu s^2/\sigma^2$ has a χ^2 distribution with ν degrees of freedom and is independent of the z_i . Dunnett (1955) has evaluated this joint density for the case of $\rho_{ij} = \rho = .5$, by obtaining $F_n(z_1, z_2, \dots, z_n; \{\rho_{ij}\})$ and integrating out s . Use of the Clark algorithm would provide a generalization of their result to the

case of general $\{\rho_{ij}\}$, a natural application of which would be a generalization of Dunnett's test to the case of unequal sample sizes among the $k + 1$ groups (i.e., treatment groups and a single control).

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Table 1

Probability that n Standard Normal Random Variables with
Common Correlation ρ , are Simultaneously $\leq h$.

A. Comparison with MULNOR

n	h	ρ	True ¹	MULNOR			Clark	
				Prob	Time ²	Time ³	Prob	Time ³
3	2.0	.9	.96170	.96170	.196	.060	.96185	.0008
4	2.0	.5	.92845	.92845	7.275	1.760	.93088	.0012
4	2.0	.8	.94759	.94758	13.735	2.913	.94819	.0012
4	2.0	.9	.95708	.95707	18.557	3.855	.95730	.0012
5 ⁴	1.0	.3	.52111	.52113	10.461	8.900	.51341	.0016
7 ⁴	0.0	.9	.32967	.32965	NA	98040	.32921	.0026
7 ⁴	0.0	.2	.04043	.04038	NA	733	.04122	.0026

¹ Gupta (1963)

² Seconds on a DEC 2060

³ Seconds on a COMPAQ 386-25, Weitek 3167, SVS FORTRAN

⁴ Accuracy set to 10^{-3} instead of 10^{-4} for MULNOR

B. Higher Dimensional Integrals

n	h	ρ	True ¹	Clark	
				Prob	Time
10	0	.5	.09091	.08907	.0044
20	0	.5	.04762	.04657	.0134
40	0	.5	.02439	.02390	.0459

¹ $F_n(0, 0, \dots, 0; \{.5\}) = \frac{1}{n+1}$

C. Tail Probabilities

n	h	ρ	True ¹	Clark
3	-2.5	.5	.00017	.00021
3	-2.5	.9	.00230	.00231
5	-2.5	.5	.00003	.00004
5	-2.5	.9	.00157	.00156
10	-2.5	.5	.00000	.00000
10	-2.5	.9	.00099	.00098

¹ Gupta (1963)

Distribution List

Dr. Terry Ackerman
Educational Psychology
210 Education Bldg.
University of Illinois
Champaign, IL 61801

Dr. James Aigler
1403 Norman Hall
University of Florida
Gainesville, FL 32605

Dr. Erling B. Andersen
Department of Statistics
Studiestræde 6
1455 Copenhagen
DENMARK

Dr. Ronald Armstrong
Rutgers University
Graduate School of Management
Newark, NJ 07102

Dr. Eva L. Baker
UCLA Center for the Study
of Evaluation
145 Moore Hall
University of California
Los Angeles, CA 90024

Dr. Laura L. Barnes
College of Education
University of Toledo
2801 W. Bancroft Street
Toledo, OH 43606

Dr. William M. Bart
University of Minnesota
Dept. of Educ. Psychology
130 Burton Hall
77 Pillsbury Dr., S.E.
Minneapolis, MN 55455

Dr. Isaac Bejar
Mail Stop 10-R
Educational Testing Service
Rosedale Road
Princeton, NJ 08541

Dr. Menucha Brenbaum
School of Education
Tel Aviv University
Ramat Aviv 69978
ISRAEL

Dr. Arthur S. Blawie
Code N722
Naval Training Systems Center
Orlando, FL 32813-7100

Dr. Bruce Blossom
Defense Manpower Data Center
39 Pacific St.
Suite 155A
Monterey, CA 93943-3221

Edt. Arnold Boeser
Secue Psychologische Onderzoek
Resrutering-En Selectiecentrum
Kwartier Koningen Aalnd
Bruijnstraat
1120 Brussels, BELGIUM

Dr. Robert Breau
Code 281
Naval Training Systems Center
Orlando, FL 32826-3224

Dr. Robert Brennan
American College Testing
Programs
P. O. Box 168
Iowa City, IA 52243

Dr. Gregory Candell
CTB/McGraw-Hill
2500 Garden Road
Monterey, CA 93940

Dr. John B. Carroll
409 Elliott Rd., North
Chapel Hill, NC 27514

Dr. John M. Carroll
IBM Watson Research Center
User Interface Institute
P.O. Box 704
Yorktown Heights, NY 10598

Dr. Robert M. Carroll
Chief of Naval Operations
OP-01B2
Washington, DC 20350

Dr. Raymond E. Chisnal
UES LAMP Science Advisor
AFHRL/MOEL
Brooks AFB, TX 78235

Mr. Hua Hua Chung
University of Illinois
Department of Statistics
101 Illini Hall
725 South Wright St.
Champaign, IL 61820

Dr. Norman Cliff
Department of Psychology
Univ. of So. California
Los Angeles, CA 90089-1061

Director, Manpower Program
Center for Naval Analyses
4401 Ford Avenue
P.O. Box 16268
Alexandria, VA 22302-0268

Director,
Manpower Support and
Readiness Program
Center for Naval Analyses
2000 North Beauregard Street
Alexandria, VA 22311

Dr. Stanley Collier
Office of Naval Technology
Code 222
300 N. Quincy Street
Arlington, VA 22217-5000

Dr. Hans F. Crombag
Faculty of Law
University of Limburg
P.O. Box 616
Maastricht
The NETHERLANDS 6200 MD

Ms. Carolyn R. Crone
Johns Hopkins University
Department of Psychology
Charles & 34th Street
Baltimore, MD 21218

Dr. Timothy Drvey
American College Testing Program
P.O. Box 168
Iowa City, IA 52243

Dr. C. M. Dayton
Department of Measurement
Statistics & Evaluation
College of Education
University of Maryland
College Park, MD 20742

Dr. Ralph J. DeAyala
Measurement, Statistics,
and Evaluation
Benjamin Bldg., Rm. 4112
University of Maryland
College Park, MD 20742

Dr. Lou DiBello
CERL
University of Illinois
103 South Mathews Avenue
Urbana, IL 61801

Dr. Deshpande Divgi
Center for Naval Analyses
4401 Ford Avenue
P.O. Box 16268
Alexandria, VA 22302-0268

Mr. Hei-Ki Dong
Bell Communications Research
Room PYA-1K207
P.O. Box 1330
Piscataway, NJ 08855-1330

Dr. Fritz Drasgow
University of Illinois
Department of Psychology
603 E. Daniel St.
Champaign, IL 61820

Dr. Stephen Dunbar
224B Lindquist Center
for Measurement
University of Iowa
Iowa City, IA 52242

Dr. James A. Earles
Air Force Human Resources Lab
Brooks AFB, TX 78235

Dr. Susan Embretson
University of Kansas
Psychology Department
426 Fraser
Lawrence, KS 66045

Dr. George Englehard, Jr.
Division of Educational Studies
Emory University
210 Fishburne Bldg.
Atlanta, GA 30322

Dr. Benjamin A. Fairbank
Operational Technologies Corp.
5825 Callaghan, Suite 225
San Antonio, TX 78228

Dr. P.A. Federico
Code 51
NPRDC
San Diego, CA 92152-6800

Dr. Leonard Feldt
Lindquist Center
for Measurement
University of Iowa
Iowa City, IA 52242

Dr. Richard L. Ferguson
American College Testing
P.O. Box 168
Iowa City, IA 52243

Dr. Gerhard Fischer
Liebiggasse 53
A 1010 Vienna
AUSTRIA

Dr. Myron Fischl
U.S. Army Headquarters
DAPE-MRR
The Pentagon
Washington, DC 20310-0300

Prof. Donald Fitzgerald
University of New England
Department of Psychology
Armidale, New South Wales 2351
AUSTRALIA

Mr. Paul Foley
Navy Personnel R&D Center
San Diego, CA 92152-6800

Dr. Alfred R. Pregly
AFOSR/NL Bldg. 410
Bolling AFB, DC 20332-6448

Dr. Robert D. Gibbons
Illinois State Psychiatric Inst.
Rm 529W
1601 W Taylor Street
Chicago, IL 60612

Dr. Janice Gifford
University of Massachusetts
School of Education
Amherst, MA 01003

Dr. Drew Gitomer
Educational Testing Service
Princeton, NJ 08541

Dr. Robert Glaser
Learning Research
& Development Center
University of Pittsburgh
3939 O'Hara Street
Pittsburgh, PA 15260

Dr. Bert Green
Johns Hopkins University
Department of Psychology
Charles & 34th Street
Baltimore, MD 21218

Michael Habon
DORNIER GMBH
P.O. Box 1430
D-7990 Friednchafen 1
WEST GERMANY

Prof. Edward Haertel
School of Education
Stanford University
Stanford, CA 94305

Dr. Ronald K. Hambleton
University of Massachusetts
Laboratory of Psychometric
and Evaluative Research
Hille South, Room 152
Amherst, MA 01003

Dr. DeWyn Hamach
University of Illinois
51 Gerty Drive
Champaign, IL 61820

Dr. Grant Henning
Senior Research Scientist
Division of Measurement
Research and Services
Educational Testing Service
Princeton, NJ 08541

Ms. Rebecca Heller
Navv Personnel R&D Center
Code 63
San Diego, CA 92152-6800

Dr. Thomas M. Hirsch
ACT
P.O. Box 168
Iowa City, IA 52243

Dr. Paul W. Holland
Educational Testing Service, 2117
Rosedale Road
Princeton, NJ 08541

Dr. Paul Horst
577 G Street, #184
Chula Vista, CA 92010

Dr. Lloyd Humphreys
University of Illinois
Department of Psychology
603 East Daniel Street
Champaign, IL 61820

Dr. Steven Hunka
3-104 Educ. N.
University of Alberta
Edmonton, Alberta
CANADA T6G 3G5

Dr. Huynh Huynh
College of Education
Univ. of South Carolina
Columbia, SC 29208

Dr. Robert Jannarone
Elec. and Computer Eng. Dept.
University of South Carolina
Columbia, SC 29208

Dr. Kumar Joag-dev
University of Illinois
Department of Statistics
101 Illini Hall
725 South Wright Street
Champaign, IL 61820

Dr. Douglas H. Jones
1280 Woodfern Court
Toms River, NJ 08753

Dr. Brian Junter
Carnegie-Mellon University
Department of Statistics
Schenley Park
Pittsburgh, PA 15213

Dr. Milton S. Katz
European Science Coordination
Office
U.S. Army Research Institute
Box 65
FPO New York 09510-1500

Prof. John A. Keau
Department of Psychology
University of Newcastle
N.S.W. 2308
AUSTRALIA

Dr. Jwa-keun Kim
Department of Psychology
Middle Tennessee State
University
P.O. Box 522
Murfreesboro, TN 37132

Mr. Soon-Hoon Kim
Computer-based Education
Research Laboratory
University of Illinois
Urbana, IL 61801

Dr. G. Gage Kingbury
Portland Public Schools
Research and Evaluation Department
501 North Dixon Street
P.O. Box 3107
Portland, OR 97209-3107

Dr. William Koch
Box 7246, Meas. and Eval. Ctr.
University of Texas-Austin
Austin, TX 78703

Dr. Richard J. Koubek
Department of Biomedical
& Human Factors
139 Engineering & Math Bldg.
Wright State University
Dayton, OH 45435

Dr. Leonard Kroeter
Navy Personnel R&D Center
Code 62
San Diego, CA 92152-6800

Dr. Jerry Labnus
Defense Manpower Data Center
Suite 400
1600 Wilson Blvd
Rosslyn, VA 22209

Dr. Thomas Leonard
University of Wisconsin
Department of Statistics
1210 West Dayton Street
Madison, WI 53705

Dr. Michael Levine
Educational Psychology
210 Education Bldg.
University of Illinois
Champaign, IL 61801

Dr. Charles Lewis
Educational Testing Service
Princeton, NJ 08541-0001

Mr. Rodney Lum
University of Illinois
Department of Psychology
603 E. Daniel St.
Champaign, IL 61820

Dr. Robert L. Lunn
Campus Box 249
University of Colorado
Boulder, CO 80309-0249

Dr. Robert Lockman
Center for Naval Analysis
4401 Ford Avenue
P.O. Box 16268
Alexandria, VA 22302-0268

Dr. Frederic M. Lord
Educational Testing Service
Princeton, NJ 08541

Dr. Richard Luecht
ACT
P.O. Box 168
Iowa City, IA 52243

Dr. George B. Macready
Department of Measurement
Statistics & Evaluation
College of Education
University of Maryland
College Park, MD 20742

Dr. Gary Marco
Stop 31-E
Educational Testing Service
Princeton, NJ 08541

Dr. Cleasen J. Martin
Office of Chief of Naval
Operations (OP 13 F)
Navv Annex, Room 2832
Washington, DC 20350

Dr. James R. McBride
The Psychological Corporation
1250 Sixth Avenue
San Diego, CA 92101

Dr. Clarence C. McCormick
HQ, USMEPCOM/MEPCT
2500 Green Bay Road
North Chicago, IL 60064

Mr. Christopher McCusker
University of Illinois
Department of Psychology
603 E. Daniel St.
Champaign, IL 61820

Dr. Robert McKinley
Educational Testing Service
Princeton, NJ 08541

University of Illinois at Chicago/Gibbons

Mr. Alan Mead
c/o Dr. Michael Levine
Educational Psychology
210 Education Bldg.
University of Illinois
Champaign, IL 61801

Dr. Timothy Miller
ACT
P. O. Box 168
Iowa City, IA 52243

Dr. Robert Mislevy
Educational Testing Service
Princeton, NJ 08541

Dr. William Montague
NPRDC Code 13
San Diego, CA 92152-6800

Ms. Kathleen Moreno
Navy Personnel R&D Center
Code 62
San Diego, CA 92152-6800

Headquarters Marine Corps
Code MPI-20
Washington, DC 20380

Dr. Ratna Nandakumar
Educational Studies
Willard Hall, Room 213E
University of Delaware
Newark, DE 19716

Dr. Harold F. O'Neil, Jr.
School of Education - WPH 801
Department of Educational
Psychology & Technology
University of Southern California
Los Angeles, CA 90089-0031

Dr. James B. Olsen
WICAT Systems
1875 South State Street
Orem, UT 84058

Dr. Judith Orasanu
Basic Research Office
Army Research Institute
5001 Eisenhower Avenue
Alexandria, VA 22333

Dr. Jesse Ortanaky
Institute for Defense Analyses
1801 N. Beauregard St.
Alexandria, VA 22311

Dr. Peter J. Pasbley
Educational Testing Service
Rosedale Road
Princeton, NJ 08541

Wayne M. Paulsen
American Council on Education
GED Testing Service, Suite 20
One Dupont Circle, NW
Washington, DC 20036

Dr. James Paulson
Department of Psychology
Portland State University
P.O. Box 751
Portland, OR 97207

Dr. Mark D. Reckase
ACT
P. O. Box 168
Iowa City, IA 52243

Dr. Malcolm Res
AFHRL/MOA
Brooks AFB, TX 78235

Mr. Steve Reiss
N660 Elliott Hall
University of Minnesota
75 E. River Road
Minneapolis, MN 55455-0344

Dr. Carl Ross
CNET-PDCD
Building 40
Great Lakes NTC, IL 60088

Dr. J. Ryan
Department of Education
University of South Carolina
Columbia, SC 29208

Dr. Fumiko Satojima
Department of Psychology
University of Tennessee
310B Austin Peay Bldg.
Knoxville, TN 37916-0900

Mr. Drew Sands
NPRDC Code 62
San Diego, CA 92152-6800

Lowell Schoer
Psychological & Quantitative
Foundations
College of Education
University of Iowa
Iowa City, IA 52242

Dr. Mary Schrauz
405 Orchid Way
Carlsbad, CA 92009

Dr. Dan Segall
Navy Personnel R&D Center
San Diego, CA 92152

Dr. Robin Shealy
University of Illinois
Department of Statistics
101 Illini Hall
725 South Wright St.
Champaign, IL 61820

Dr. Kazuo Shigemasa
7-9-24 Kugenuma-Kaigan
Fujisawa 251
JAPAN

Dr. Richard E. Snow
School of Education
Stanford University
Stanford, CA 94305

Dr. Richard C. Sorenson
Navy Personnel R&D Center
San Diego, CA 92152-6800

Dr. Judy Spray
ACT
P.O. Box 168
Iowa City, IA 52243

Dr. Martha Stocking
Educational Testing Service
Princeton, NJ 08541

Dr. Peter Stoloiff
Center for Naval Analysis
4401 Ford Avenue
P.O. Box 16268
Alexandria, VA 22302-0268

Dr. William Stout
University of Illinois
Department of Statistics
101 Illini Hall
725 South Wright St.
Champaign, IL 61820

Dr. Harbaran Swensonathan
Laboratory of Psychometric and
Evaluation Research
School of Education
University of Massachusetts
Amherst, MA 01003

Mr. Brad Sympton
Navy Personnel R&D Center
Code 62
San Diego, CA 92152-6800

Dr. John Tangney
AFOSR/NL Bldg. 410
Bolling AFB, DC 20332-6448

Dr. Kikumi Tatsuoka
Educational Testing Service
Mail Stop 03-T
Princeton, NJ 08541

Dr. Maurice Tatsuoka
Educational Testing Service
Mail Stop 03-T
Princeton, NJ 08541

Dr. David Thissen
Department of Psychology
University of Kansas
Lawrence, KS 66044

Mr. Thomas J. Thomas
Johns Hopkins University
Department of Psychology
Charles & Math Street
Baltimore, MD 21218

Mr. Gary Thomeason
University of Illinois
Educational Psychology
Champaign, IL 61820

Dr. Robert Toulakian
University of Missouri
Department of Statistics
222 Math. Sciences Bldg.
Columbia, MO 65211

Dr. Ledyard Tucker
University of Illinois
Department of Psychology
403 E. Daniel Street
Champaign, IL 61820

Dr. David Vale
Assessment Systems Corp.
2233 University Avenue
Suite 440
St. Paul, MN 55114

Dr. Frank L. Viano
Navy Personnel R&D Center
San Diego, CA 92152-6800

Dr. Howard Weiner
Educational Testing Service
Princeton, NJ 08541

Dr. Michael T. Waller
University of Wisconsin-Milwaukee
Educational Psychology Department
Box 413
Milwaukee, WI 53201

Dr. Ming-Mei Wang
Educational Testing Service
Mail Stop 03-T
Princeton, NJ 08541

Dr. Thomas A. Warr
FAA Academy AAC934D
P.O. Box 25082
Oklahoma City, OK 73125

Dr. Brian Waters
HUMRRO
1100 S. Washington
Alexandria, VA 22314

Dr. David J. Weiss
N660 Elliott Hall
University of Minnesota
75 E. River Road
Minneapolis, MN 55455-0344

Dr. Ronald A. Weitzman
Box 146
Carmel, CA 93921

Major John Weisb
AFHRL/MOAN
Brooks AFB, TX 78223

Dr. Douglas Wetzel
Code 51
Navy Personnel R&D Center
San Diego, CA 92152-0800

Dr. Rand R. Wilcox
University of Southern
California
Department of Psychology
Los Angeles, CA 90089-1061

German Military Representative
ATTN: Wolfgang Wildgrube
Strenzkefeest
D-5300 Bonn 2
4000 Brandynne Street, NW
Washington, DC 20016

Dr. Bruce Williams
Department of Educational
Psychology
University of Illinois
Urbana, IL 61801

Dr. Hilda Wing
Federal Aviation Administration
900 Independence Ave. SW
Washington, DC 20591

Mr. John H. Wolfe
Navy Personnel R&D Center
San Diego, CA 92152-0800

Dr. George Wong
Biostatistics Laboratory
Memorial Sloan-Kettering
Cancer Center
1275 York Avenue
New York, NY 10021

Dr. Wallace Wuileck, III
Navy Personnel R&D Center
Code 51
San Diego, CA 92152-0800

Dr. Kentaro Yamamoto
02-T
Educational Testing Service
Rosedale Road
Princeton, NJ 08541

Dr. Wendy Yen
CTB/McGraw Hill
Del Monte Research Park
Monterey, CA 93940

Dr. Joseph L. Young
National Science Foundation
Room 320
1800 G Street, N.W.
Washington, DC 20550

Mr. Anthony R. Zars
National Council of State
Boards of Nursing, Inc.
625 North Michigan Avenue
Suite 1544
Chicago, IL 60611